Long- and short-range correlations in the *ab-initio* no-core shell model

Ionel Stetcu* and Bruce R. Barrett
Department of Physics, University of Arizona, P.O. Box 210081, Tucson, Arizona 85721, USA

Petr Navrátil
Lawrence Livermore National Laboratory, Livermore, P.O. Box 808, California 94551, USA

James P. Vary
Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011, USA

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In the framework of the *ab-initio* no-core shell model (NCSM), we describe the longitudinal-longitudinal distribution function, part of the inclusive (e, e') longitudinal response. In the two-body cluster approximation, we compute the effective operators consistent with the unitary transformation used to obtain the effective Hamiltonian. When short-range correlations are probed, the results display independence from the model space size and length scale. Long-range correlations are more difficult to model in the NCSM and they can be described only by increasing the model space or increasing the cluster size. In order to illustrate the model space independence for short-range observables, we present results for a large set of model spaces for ^{4}He, and in $0{-}4\hbar\Omega$ model spaces for ^{12}C.

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Atomic nuclei are the result of a delicate interplay between short- and long-range correlations among the nucleons, which makes their theoretical description rather challenging. For light nuclei, very successful methods, such as Green's function Monte Carlo [1], hyperspherical harmonics [2], and the no-core shell model (NCSM) [3–7], have been developed recently. They allow an *ab-initio* description of nuclear properties, the only ingredients being realistic nucleon-nucleon (*NN*) interactions, which describe the experimental phaseshifts with high accuracy, and theoretical three-nucleon forces.

In the *ab initio* NCSM, one starts with a realistic *NN* interaction (theoretical three-body forces can also be used, but we will not discuss this case here) and performs a unitary transformation [8–10] to a model space, which allows an exact diagonalization in a finite many-body space, defined by the number of excitations above a mean-field-like configuration. Details of the procedure are available to the interested reader in previous publications [3–6]. Recently, we have extended the same procedure from the Hamiltonian to general one- and two-body operators [11–13]. The effect of the procedure is to reduce the dependence of the observables upon the model space and harmonic oscillator (HO) frequency, and, in the lowest approximation, it has proven to be effective only for short-range operators [12].

Using the unitary transformation approach [8–10], we obtain the following expression for the effective operators [8,14]

$$P\mathcal{O}P = \frac{P + P\omega^\dagger Q}{\sqrt{P+\omega^\dagger\omega}}\, O\, \frac{P + Q\omega P}{\sqrt{P+\omega^\dagger\omega}}, \tag{1}$$

where the transformation operator ω satisfies the condition $Q\omega P = \omega$, with P and Q the projector operators in the model and complementary spaces, respectively, and O is the bare general operator, which acts in the entire space.

In principle, the transformation operator ω can be computed using a finite set of eigenvectors in the full space, making use of the overlap of the full space eigenvectors with the basis states in the P and Q spaces [4,5], i.e.,

$$\langle\alpha_Q|\omega|\alpha_P\rangle = \sum_{k\in\mathcal{K}} \langle\alpha_Q|k\rangle\langle\tilde{k}|\alpha_P\rangle. \tag{2}$$

In the last equation, $|\alpha_P\rangle$ and $|\alpha_Q\rangle$ are the basis states in the P and Q spaces, respectively. The summation runs over a finite subset, $\mathcal{K}$, of eigenvectors in the full space, and the tilde stands for the inverse of the overlap matrix, i.e., $\sum_{\alpha_P}\langle k'|\alpha_P\rangle\langle\alpha_P|\tilde{k}\rangle = \delta_{kk'}$.

Equation (2) shows that in order to obtain the transformation operator ω one needs the solution to the initial A-body problem. This makes its application impractical, unless we use approximations. In the simplest approximation, the transformation operator ω and, therefore, the effective interaction are obtained in the relative system of two particles, in a large HO basis. The Q space is chosen to be a few hundred $\hbar\Omega$ excitations in order to obtain an exact solution to the two-body Schrödinger equation. Due to the rotational symmetry, we formulate the problem in two-nucleon channels with good total spin s, total angular momentum j, and isospin t, reducing drastically the dimensions involved, when performing the summation over the states in the Q space in Eq. (1). The same procedure can be applied to operators that can be analytically expressed in terms of relative and center-of-mass coordinates of pairs. However, note that in the case of non-scalar operators calculations performed with Eq. (1) become more difficult, because such operators can in general couple different channels. As

*On leave from the National Institute for Physics and Nuclear Engineering "Horia Hulubei," Bucharest, Romania.

expected, since the transformation operator is a scalar, this procedure changes neither the character nor the rank of the bare operator. By construction, keeping the cluster approximation fixed (in this case, the two-body cluster) and increasing the model space decreases the effect of the renormalization. This was demonstrated in earlier papers in the case of ^{3}H for the ground-state energy [7], and in this paper we will also demonstrate this by comparisons between the effective and bare results for an observable related to the Coulomb sum rule.

The inclusive (e, e') longitudinal data presents one of the clearest experimental signatures for short-range correlations in the wave-function of the ground state, at least for light nuclei. The Coulomb sum rule

$$S_L(q) = \frac{1}{Z}\int_{\omega_{\mathrm{el}}}^{\infty} d\omega S_L(q,\omega) \qquad (3)$$

is the total integrated strength measured in electron scattering. In Eq. (3), $S_L(q,\omega) = R(q,\omega)/|G_{E,p}(q,\omega)|^2$, with $R(q,\omega)$ the longitudinal response function and $G_{E,p}(q,\omega)$ the proton electric form factor, while ω_{el} is the energy of the recoiling A-nucleon system with Z protons. The Coulomb sum rule $S_L(q)$, which is related to the Fourier transform of the proton-proton distribution function [15], can be expressed as [16]

$$\begin{aligned} S_L(q) &= \frac{1}{Z}\langle \mathrm{g.s.}|\rho_L^\dagger(\mathbf{q})\rho_L(\mathbf{q})|\mathrm{g.s.}\rangle - \frac{1}{Z}|\langle \mathrm{g.s.}|\rho_L(\mathbf{q})|\mathrm{g.s.}\rangle|^2 \\ &\equiv 1 + \rho_{LL}(q) - ZF_L(q)/G_{E,p}(q,\omega_{\mathrm{el}}), \end{aligned}$$

where $F_L(q)$ is the longitudinal form factor. If one neglects the relativistic corrections and two-body currents, $\rho_L(\mathbf{q})$ is simply the charge operator

$$\rho_L(\mathbf{q}) = \frac{1}{2}\sum_{i=1}^{A}\exp(i\mathbf{q}\cdot\mathbf{r}_i)(1+\tau_{z,i}).$$

Consequently, the longitudinal-longitudinal distribution function becomes [16]

$$\rho_{LL}(q) = \frac{1}{4Z}\sum_{i\neq j}\langle \mathrm{g.s.}|j_0(q|\mathbf{r}_i-\mathbf{r}_j|)(1+\tau_{z,i})(1+\tau_{z,j})|\mathrm{g.s.}\rangle.$$

We present the results for $\rho_{LL}(q)$ for ^{4}He in Figs. 1 and 2. We have limited this investigation to two-body interactions only, and, in particular, have used the phenomenological CD-Bonn NN force [17], because it yields reasonable convergence properties with increasing the size of the model space. Although experimental data for the longitudinal-longitudinal distribution function exist, a direct comparison with experiment is not suitable, because we neglect: on one hand, (i) three-body forces in the model Hamiltonian, and, on the other hand, (ii) exchange currents and (iii) relativistic corrections for the charge operator. Nevertheless, the results demonstrate the behavior of short- and long-range operators within the framework of the NCSM.

Using a Gaussian operator of variable range, we have shown previously how the renormalization of this two-body operator depends upon its range [12]. We found that a short-range two-body operator is renormalized accurately at the two-body cluster level, while a long-range operator is weakly renormalized. The same behavior can also be inferred from Fig. 1, where we present $\rho_{LL}(q)$ calculated in two model spaces for a fixed frequency, using both bare and effective operators. Thus, at large momentum transfer, the use of effective operators produces model-space independent results. Even in small model spaces we obtain good results, although Fig. 3 shows that the ground-state wave function is not fully converged in such small spaces, since the ground-state enegy is not converged to the exact value. In particular, for $N_{\max} = 10$ (or $10\hbar\Omega$, in terms of allowed excitations beyond the lowest configuration) the ground-state energy is -28.30 MeV for $\hbar\Omega = 19$ MeV and -27.56 MeV for $\hbar\Omega = 28$ MeV, compared to the exact ^{4}He CD-Bonn ground-state

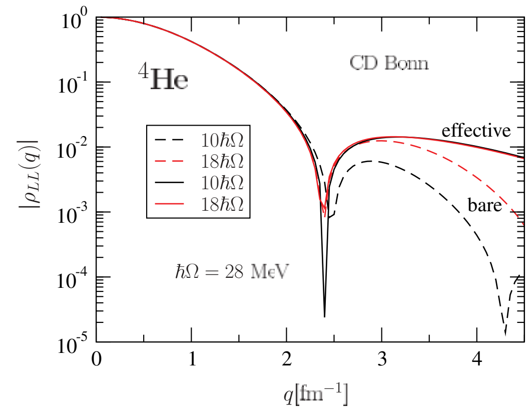

FIG. 1. (Color online) The longitudinal-longitudinal distribution function $\rho_{LL}(q)$ in ^{4}He for two model spaces ($10\hbar\Omega$ and $18\hbar\Omega$) and fixed frequency $\hbar\Omega = 28$ MeV, using bare (dashed curves) and effective (continuous curves) operators. As discussed in the text, the results obtained with effective operators are almost indistinguishable.

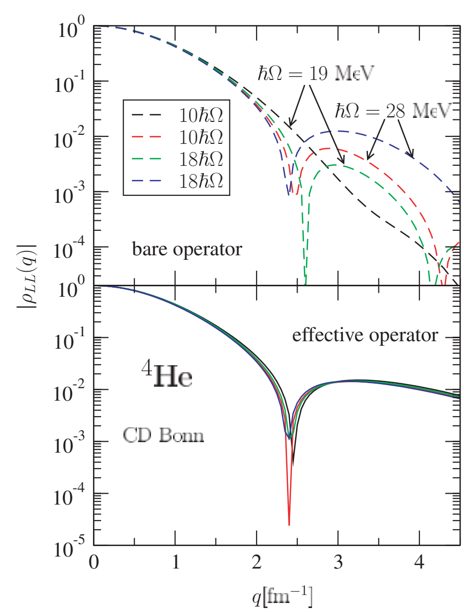

FIG. 2. (Color online) Longitudinal-longitudinal distribution function, using bare (upper panel) and effective (lower panel) operators. We used two different HO frequencies, 19 MeV and 28 MeV, and two model spaces, $10\hbar\Omega$ and $18\hbar\Omega$.

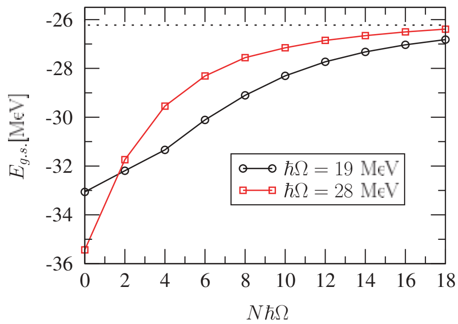

FIG. 3. (Color online) The convergence of the ground-state energy for the two frequencies used to compute the $\rho_{LL}(q)$. The dotted line is the exact ground-state energy for the CD-Bonn interaction (−26.16 MeV [18]).

energy of −26.16 MeV [18]. The complete convergence of the ground-state energy can be obtained within the NCSM, as demonstrated, e.g., in Fig. 1 of Ref. [19]. As expected, Fig. 1 shows that in the large model space the renormalization is weaker, i.e., there is less need for renormalization, so that the value obtained with the bare operator is similar to the value obtained with the renormalized operator. Thus, for $q \lesssim 3$ fm^{-1} one cannot distinguish between the results obtained using bare operators in the 18$\hbar\,\Omega$ model space for HO frequency $\hbar\,\Omega = 28$ MeV and the ones obtained using effective operators. For momenta $q > 3$ fm^{-1} the results using the bare operator deviate from the renormalized values, because the short-range correlations induced by the interactions are cast into the effective interaction. If one wants to account for short-range correlations using a bare short-range operator, one has to increase the model space, so that the effect of the short-range renormalization is negligible. However, such a scheme would require a vast number of $\hbar\,\Omega$ excitations to obtain a convergent result.

In Fig. 2, we present $\rho_{LL}(q)$ calculated in 10$\hbar\,\Omega$ and 18$\hbar\,\Omega$ model spaces, with HO frequencies of 19 and 28 MeV. In the upper panel we show the results obtained using bare operators. In this case, the values are spread over orders of magnitude. In contrast, the lower panel demonstrate independence of *both* model space and frequency, when using the appropriate effective operator, although the ground-state energy is not converged, as illustrated in Fig. 3. Moreover, Fig. 2 shows that the convergence depends strongly upon the HO frequency, when using bare operators. Thus, the results obtained with the bare operator in 18$\hbar\,\Omega$ with $\hbar\,\Omega = 19$ MeV are far from the results using effective operators; moreover, this curve shows a second minimum around $q \simeq 4.25$ fm$^{-1,}$ whereas the converged results are almost flat and several orders of magnitude larger for this value of the momentum transfer. In contrast, even if still significantly different from the converged values, the results for $\hbar\,\Omega = 28$ MeV are closer to the ones obtained with effective operators.

One can better observe the influence of the frequency and model space in Fig. 4, where we present the results for ^{12}C. For ^{12}C, unlike the case of ^{4}He, where we have used a Jacobi-coordinate HO basis (see, e.g., Ref. [7]), the investigation was performed using the MANY-FERMION DYNAMICS code [20], which employs a Slater determinant basis

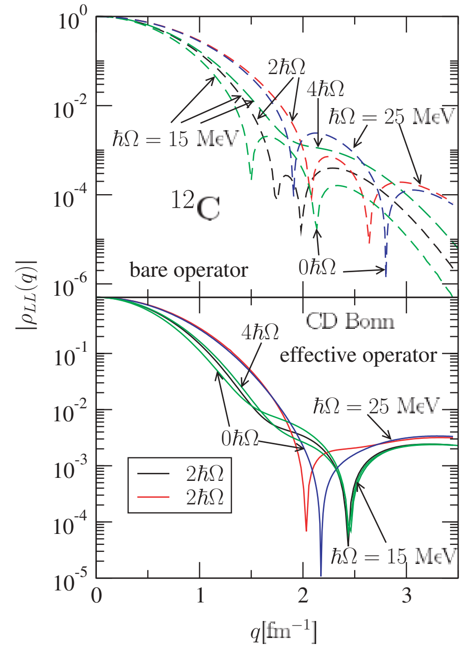

FIG. 4. (Color online) Longitudinal-longitudinal distribution function for different model spaces and frequencies in ^{12}C, using bare (upper panel) and effective (lower panel) operators. For the 4$\hbar\,\Omega$ model space, we show only the results using $\hbar\,\Omega = 15$ MeV. While the frequency dependence is not completely removed, the use of effective operators produces indistinguishable results at large q for different model spaces, as discussed in the text.

and becomes much more efficient for $A > 5$ than a Jacobi-coordinate approach. In this case, the number of many-body configurations increases very rapidly and one has to limit the truncation to a smaller model space. We present results for up to 4$\hbar\,\Omega$ model spaces. Again, note in the upper panel that the results obtained with the bare operators differ widely in shape and magnitude. When using effective operators, however, all curves collapse into the same shape and agree with each other for $q \gtrsim 3$ fm^{-1}, as shown in the lower panel. Because the calculation is not fully converged, the minima still change significantly with frequency and model space, even when one uses effective operators. One observes that, although the results at high momentum transfer are very close together, a small dependence upon the HO frequency persists.

In summary, we have investigated the longitudinal-longitudinal distribution function (part of the Coulomb sum rule) in the framework of the NCSM, utilizing the two-body cluster approximation. Thus, we have extended our previous application of the effective operator formalism [11–13] to the calculation of an observable that probes the short-range correlations. We find that even very small model spaces can provide an accurate description of the short-range observables, *if* effective operators are employed. This investigation shows that reliable results can be obtained for short-range operators, even for heavier nuclei, such as ^{12}C, for which the 0$\hbar\,\Omega$ results are accurate at higher q. As expected, intermediate- and long-range correlations can be best described by increasing the size of the model space and/or by a using higher order cluster approximation.

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